



What is claimed is:

1. An apparatus for performing spectral analysis, the apparatus comprising:
  - a. a data acquisition system configured to measure a signal emitted from a sample in response to excitation energy applied thereto, and to average the measured signal over a plurality of measurements to generate an averaged signal;
  - b. a data processing system including:
    - a noise-reduction pre-processor configured to create a vector space from said averaged signal, and to generate the singular values and corresponding eigenvectors of a correlation matrix constructed within said vector space, said vector space containing a noise-free signal subspace and a noise subspace, said singular values including noise-free singular values associated with said noise-free signal subspace, and noise singular values associated with said noise subspace; and
    - c. a control system configured to identify a gap between a noise-free singular value and an adjacent noise singular value, so as to request the data acquisition system to perform additional measurements if no such separation can be identified, and to prevent further measurements from being made by the data acquisition system if the appearance and stability of said gap can be established.
2. An apparatus in accordance with claim 1, wherein said spectral analysis comprises an NMR spectral analysis, said excitation energy comprises RF excitation pulses, and said measured signal comprises an NMR transient.
3. An apparatus in accordance with claim 1, wherein said control system comprises:
  - a. a graphics system adapted to generate a plot of said singular values;

- b. a pattern recognition system adapted to identify a gap in said plot between said noisefree singular value and said adjacent noise singular value, and to verify the stability of said gap; and
- c. a command signal generator, responsive to said pattern recognition system, configured to generate an output signal requesting for more measurements from said data acquisition system, in the absence of an identifiable gap, and to generate an output signal requesting that further measurements be discontinued, if the appearance and the stability of said gap has been established by said pattern recognition system.

4. An apparatus in accordance with claim 1, wherein said noise-reduction preprocessor comprises:

- a. a matrix generator configured to form a vector space from the averaged signal and constructing a correlation matrix within the vector space, the vector space containing a noisefree signal subspace and a noise subspace;
- b. a matrix diagonalizer configured to diagonalize the correlation matrix to obtain its singular values and the corresponding eigenvectors, the singular values including noisefree singular values associated with the noisefree signal subspace, and noise singular values associated with the noise subspace; and
- c. a signal projector configured to project the averaged signal onto the noisefree subspace to generate a noise-reduced signal.

5. An apparatus in accordance with claim 4, wherein said data processing system further comprises a spectral estimator for generating a spectrum by converting said noise-reduced signal into a frequency domain.

6. An apparatus in accordance with claim 1, wherein said data acquisition system is configured to sample each measured signal with a sampling period  $\tau$ , and to average the corresponding sample points over said plurality of measurements, so as to store said averaged signal as a discretized set of  $N$  data points  $c_n$  ( $n = 0, \dots, N-1$ ).

## 7. An apparatus in accordance with claim 6,

wherein said data processing system is configured to store each data point  $c_n$  as a noisefree component  $x_n$  ( $n = 0, \dots, N-1$ ) and a noise component  $\epsilon_n$  ( $n = 0, \dots, N-1$ ), and to store each noisefree component  $x_n$  as a finite sum of damped complex harmonics weighted by respective coefficients.

## 8. An apparatus in accordance with claim 7,

wherein said sum is over a number  $K$  of said damped complex harmonics, so that each noisefree component  $x_n$  can be stored as:

$$x_n = \sum d_k \exp (-iw_k \tau n)$$

where  $d_k$  represents the weighting coefficient of the  $k$ -th damped complex harmonics, and  $w_k$  represents the complex frequency of the  $k$ -th damped complex harmonics.

## 9. An apparatus in accordance with claim 1, wherein said data acquisition system further comprises a windowing subsystem configured to apply a windowing filter to a Fourier transform of said averaged signal, so as to generate one or more decimated signals having a limited bandwidth.

## 10. An apparatus in accordance with claim 9,

wherein said data processing system is configured to store the inverse Fourier transform of each decimated signal as a set of  $N_d$  decimated data points  $c_n^d$  ( $n = 0, \dots, N_d-1$ ),

and wherein said set of decimated data points have a signal length  $N_d$  that is substantially less than  $N$  and a sampling period  $\tau_d$  that is substantially greater than  $\tau$ .

## 11. An apparatus in accordance with claim 10,

wherein said vector space created by said noise-reduction pre-processor comprises an  $M$ -dimensional vector space defined by a number  $N_d - M + 1$  of linearly independent  $M$ -dimensional vectors, and

wherein said data processing system is configured to store said M-dimensional vectors in a form given by:

$$c_n^d = (c_n^d, c_{n+1}^d, \dots, c_{n+M-1}^d),$$

where  $c_n^d$  represent said decimated data points.

12. A system in accordance with claim 11, wherein said correlation matrix constructed by said matrix generator is Hermitian and covariant, and has a dimension MxM, and wherein said correlation matrix is formed from said M-dimensional vectors and in accordance with a formula given by:

$$R_{ij} = 1 / (N_d - M + 1) \sum c_{n+i-1} c_{n+j-1}^*$$

13. A system in accordance with claim 11, wherein said projection of said averaged signal by said signal projector is based on a projection formula given by:

$$\bar{c}_n^{nr} = \sum_{k=1}^K (\bar{u}_k^*, \bar{c}_n) \bar{u}_k$$

where  $u_k$  represent said eigenvectors corresponding to said singular values.

14. A control system for controlling the acquisition and processing of data by an NMR apparatus so as to reduce the NMR data acquisition time required to generate a noise-reduced NMR spectrum, said NMR apparatus comprising a data acquisition system for measuring NMR response signals and averaging said response signals over a plurality of measurements, and a data processing system for processing said NMR response signals by extracting the singular values and the corresponding eigenvectors of a harmonic inversion correlation matrix formed in a vector space defined by data points sampled from said averaged signals, said vector space containing a noisefree signal subspace and a noise subspace, said control system comprising:

- a. a first processing system for identifying a gap between a noisefree singular value, associated with said noisefree signal subspace, and an adjacent noise singular value, associated with said noise subspace, so that said control system can request further measurements by said data acquisition system if said gap cannot be identified; and

b. a second processing system for determining the stability of said gap, so that said control system can request further measurements by said data acquisition system if said gap has not stabilized, and can discontinue any further measurements by said data acquisition system, if said gap has stabilized.

15. A control system for controlling the acquisition and processing of data by a spectral analysis apparatus so as to reduce the data acquisition time required to generate a noise-reduced spectrum, said apparatus comprising a data acquisition system for measuring response signals from a sample and averaging the response signals over a plurality of measurements, and a data processing system for processing said response signals by extracting the singular values and the corresponding eigenvectors of a harmonic inversion correlation matrix formed in a vector space defined by said averaged signals, said vector space containing a noisefree signal subspace and a noise subspace, said control system comprising:

a. a computer-readable medium having stored therein computer-readable instructions for a processor, wherein said instructions when executed by said processor cause said processor to:

- 1) identify a gap between a noisefree singular value, associated with said noisefree signal subspace, and an adjacent noise singular value, associated with said noise subspace;
- 2) request further measurements by said data acquisition system if said gap cannot be identified;
- 3) if said gap appears, determine the stability of said gap; and
- 4) request further measurements by said data acquisition system, if said gap does not stabilize, and request that no further measurements be made by said data acquisition system, if said gap has stabilized.

16. A data processing system for processing NMR response signals measured by an NMR data acquisition system, said NMR data acquisition system comprising an NMR transmitter for delivering RF excitation pulses to an NMR sample, an NMR

receiver for detecting the response signals emitted by said NMR sample in response to said excitation pulses, and a measurement system for measuring said response signals and averaging said response signals over a plurality of measurements, said data processing system comprising:

- a. a noise-reduction pre-processor including: 1) a matrix generator for forming a vector space from said averaged signal and constructing a correlation matrix within said vector space, said vector space containing a noise-free signal subspace and a noise subspace; 2) a matrix diagonalizer for diagonalizing said correlation matrix to obtain its singular values and the corresponding eigenvectors, said singular values including noise-free singular values associated with said noise-free signal subspace, and noise singular values associated with said noise subspace; and 3) a signal projector for projecting said averaged signal onto said noise-free subspace to generate a noise-reduced signal; and
- b. a spectral estimator for generating a spectrum by converting said noise-reduced signal into a frequency domain; and
- c. a control system configured to identify a separation between a noise-free singular value and an adjacent noise singular value, so as to allow the data acquisition system to perform additional measurements if no such separation can be identified, and to discontinue further measurements by the data acquisition system if the appearance and stability of said separation can be established.

17. A computer-readable medium having stored therein computer-readable instructions for a processor, wherein said instructions when executed by said processor cause said processor to:

- a. input and store a signal generated by a data acquisition system configured to measure said signal and average said signal over a plurality of measurements;
- b. compute and store a set of singular values, said singular values corresponding to the real, non-negative eigenvalues of a correlation matrix

constructed within a vector space created from said signal, said vector space containing a noisefree signal subspace and a noise subspace, said singular values including noisefree singular values associated with said noisefree signal subspace, and noise singular values associated with said noise subspace;

- c. determine whether a gap appears between a noisefree singular value and an adjacent noise singular value in a plot of said singular values, and if so, whether said gap stabilizes over one or more additional measurements of said signal;
- d. request further measurements by said data acquisition system, if said gap cannot be identified or if said gap does not stabilize; and
- e. command the data acquisition system to discontinue any further measurements, if the appearance and stability of said gap can be established.

18. A method of reducing data acquisition time in generating a spectrum, the method comprising:

- a. averaging over a number of data measurements to generate an averaged signal;
- b. constructing a correlation matrix from said averaged signal in a vector space defined using said averaged signal, said vector space including a noisefree signal subspace and a noise subspace;
- c. diagonalizing said correlation matrix to obtain the singular values and their corresponding eigenvectors, said singular values including noisefree singular values derived from said noisefree signal subspace, and noise singular values derived from said noise subspace; and
- d. determining when a gap between a noisefree singular value and a noise singular appears and stabilizes, to establish that a sufficient number of data measurements have been performed so that measurements can discontinue.

19. A method of generating a spectrum, the method comprising:

- a. measuring one or more response signals emitted by a sample in response to excitation applied thereto;
- b. averaging corresponding sample points in a plurality of signal measurements to generate a plurality of signal averaged sample points;
- c. using said signal averaged sample points to form a vector space that comprises a noisefree signal subspace and a noise subspace;
- d. constructing a correlation matrix within said vector space and diagonalizing said correlation matrix to obtain the singular values and their corresponding eigenvectors, said singular values including noisefree singular values associated with said noisefree signal subspace, and noise singular values associated with said noise subspace;
- e. determining when a gap appears between a smallest one of said noisefree singular values and a first one of said noise singular values, in a plot of said singular values, and whether said gap remains substantially stable after a plurality of iterations of steps a to d, to establish that a sufficient number of measurements has been reached for generating a substantially stable spectrum.

20. A method in accordance with claim 19, wherein said spectrum comprises an NMR spectrum, and said data measurements comprise NMR transient acquisitions.

21. A method of reducing data acquisition time in generating a spectrum, the method comprising:

- a. receiving a set of singular values from a data acquisition system, said singular values representing the eigenvalue solutions of a correlation matrix constructed from a vector space creating using one or more response signals that have been averaged over a plurality of measurements, said vector space containing a noisefree signal subspace and a noise subspace, said singular values including noisefree singular values associated with said

noisefree signal subspace and a noise subspace associated with said noise subspace;

- b. determining whether a gap appears between a noisefree singular value and an adjacent noise singular value in a plot of said singular values, and if so, whether said gap stabilizes over one or more additional measurements of said signal;
- c. requesting further measurements by said data acquisition system, if said gap cannot be identified or if said gap does not stabilize; and
- d. commanding said data acquisition system to discontinue any further measurements, if the appearance and stability of said gap can be established.

22. A method in accordance with claim 21, wherein steps b, c, and d are implemented by an operator of a control system.

23. A method in accordance with claim 21, wherein steps b, c, and d are implemented by a processor upon execution by said processor of computer-usuable instructions stored on a computer-usuable medium.

24. A method for reducing noise in spectral analysis, the method comprising:

- a. applying one or more excitation pulses to a sample and measuring a response signal therefrom;
- b. repeating step a. a plurality of times, and storing for each of said repetitions an acquired transient;
- c. sampling each transient and averaging over all of said sampled transients to generate a collection of data points  $c_n$  ( $n = 1, \dots, N$ );
- d. forming an M-dimensional vector space using said sampled data points  $c_n$  ( $n = 1, \dots, N$ ), said M-dimensional vector space comprising a noisefree signal subspace and a noise subspace;
- e. constructing an  $M \times M$  correlation matrix within said M-dimensional vector space, and diagonalizing said correlation matrix so as to extract therefrom a

set of singular values

$$u_i ( i = 1, \dots, M );$$

- f. generating a plot of said singular values  $u_i$  in M-space, said plot showing both noisefree singular values and noise singular values, wherein said noisefree singular values are associated with said noisefree signal subspace, and said noise singular values are associated with said noise subspace;
- g. determining whether a gap appears between a smallest one of plotted noisefree singular values and the first one of said plotted noise singular values;
- h. said gap does not appear, repeating steps a to g one or more times until said gap can be identified;
- i. determining whether said gap remains stable after a plurality of iterations of steps a to g; and
- j. upon stabilization of said gap, converting said sampled data points into a frequency domain so as to generate a noise-reduced spectrum.